QSAR TOOLBOX

The OECD QSAR Toolbox for Grouping Chemicals into Categories

User manual

Toolbox 3.3.5 Release Notes

Document history

Version	Comment
Version 1.0	July 2015: Toolbox 3.3.5 Release Notes

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If you have questions or comments that relate to this document, please send them to ehscont@oecd.org or visit the QSAR Toolbox discussion forum at https://community.oecd.org/community/toolbox_forum

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1 Overview

The Toolbox 3.3.5 installation is a minor update of Toolbox 3.3.2. It is available as a patch to be installed over previous version 3.3.2 install as well as a full package for fresh installations.

2 System Requirements

Minimum system requirements

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OS: Windows XP

CPU: Core 2 duo at 1.8 GHz or equivalent AMD CPU

RAM: At least 3GB of RAM

HDD: 14 GB free hard drive space

File system: NTFS

Recommended system requirements

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OS: Windows 7 64 bit or newer

CPU: I5 at 2.4GHz or faster processor or equivalent AMD CPU

RAM: 6 GB of RAM

HDD: 20 GB free hard drive space

File system: NTFS

3 Change log

I. New scientific features

1. DART scheme – correcting the boundaries of Category 8a (Aromatic compounds with alkyl, multi-halogen and nitro groups/Toluene and small alkyl toluene derivatives) by adjusting the carbon chain length
2. Endpoint vs. Endpoint improvements
3. Added export of chemical IDs.

II. Bug fixes

1. Save/Load Workflow bugs
2. Visualization problems in Data gap filling
3. Fixed a bug whereby Toolbox won't start if there is no local “My Documents” folder set
4. Various non critical bugs in Data gap filling
5. Fixed a bug when importing very large datasets
6. Fixed a "does not fall in domain" incorrect statement in the report

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